

Condensate statistics in interacting Bose gases: exact results

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Recently, a Quantum Monte Carlo method alternative to the Path Integral Monte Carlo method was developed for the numerical solution of the N -boson problem; it is based on the stochastic evolution of classical fields. Here we apply it to obtain exact results for the occupation statistics of the condensate mode in a weakly interacting trapped one-dimensional Bose gas. The temperature is varied across the critical region down to temperatures lower than the trap level spacing. We verify that the number-conserving Bogoliubov theory gives accurate predictions provided that the non-condensed fraction is small.

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The first achievement of Bose-Einstein condensation in weakly interacting atomic gases in 1995 has renewed the interest on basic aspects of the Bose-Einstein condensation phase transition [1]. In particular, an intense theoretical activity has been recently devoted to the study of the occupation statistics of the condensate mode: although no experimental result is available yet, we expect that it would provide a crucial test for many-body theories since, contrarily to more common one-body observables like the density, it involves arbitrarily high order correlation function of the quantum Bose field. While there are now well established results for the ideal Bose gas [2], calculations for the weakly interacting Bose gas have been performed within the framework of mean-field approximation only [3, 4, 5]. The intermediate regime around the critical temperature where the mean-field theory fails has therefore been left unexplored. Some controversy is still open about the validity of the Bogoliubov approach even at temperatures much lower than the critical temperature [6]. In the absence of experimental results, it is then very interesting to have exact theoretical results on the statistics of condensate occupation.

There exists an exact analytical solution to the bosonic N body problem [7], but it is restricted to the spatially homogeneous one-dimensional case. From the side of numerics, the Quantum Monte Carlo method based on the Path Integral Monte Carlo technique is in principle able to give exact predictions for any observable of the gas [8] and was successfully used to calculate the mean condensate occupation [9] and the critical temperature [10]. In the Path Integral formulation, however, the position representation is privileged which makes the calculation of highly non-local observables like the condensate occupation probabilities rather involved.

In this paper, we use instead a recently developed Quantum Monte Carlo method based on the stochastic evolution of classical fields [11, 12]. This new method has a much broader range of applicability than the standard Path Integral Monte Carlo technique: it can be applied to bosonic systems with complex wavefunctions, and even

to interacting Fermi systems [13]. As compared to the Positive- P method of quantum optics [14], it has the decisive advantage of having been proven to be convergent. In this paper, we perform the first non-trivial application of this new method, calculating for the first time the exact distribution function of the number of condensate particles in the presence of interactions, for temperatures across the Bose-Einstein condensation temperature.

An ultracold trapped interacting Bose gas in D dimensions can be modelled in a second-quantization formalism by the Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{k}} \frac{\hbar^2 \mathbf{k}^2}{2m} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \frac{g_0}{2} \sum_{\mathbf{r}} dV \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) + \sum_{\mathbf{r}} dV U_{\text{ext}}(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}); \quad (1)$$

the spatial coordinate \mathbf{r} runs on a discrete orthogonal lattice of \mathcal{N} points with periodic boundary conditions; V is the total volume of the quantization box and $dV = V/\mathcal{N}$ is the volume of the unit cell of the lattice. $U_{\text{ext}}(\mathbf{r})$ is the external trapping potential, m is the atomic mass and interactions are modeled by a two-body discrete delta potential with a coupling constant g_0 . The field operators $\hat{\Psi}(\mathbf{r})$ satisfy the usual Bose commutation relations $[\hat{\Psi}(\mathbf{r}), \hat{\Psi}^\dagger(\mathbf{r}')] = \delta_{\mathbf{r},\mathbf{r}}/dV$ and can be expanded on plane waves according to $\hat{\Psi}(\mathbf{r}) = \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}}/\sqrt{V}$ with \mathbf{k} restricted to the first Brillouin zone of the reciprocal lattice. In order for the discrete model to correctly reproduce the underlying continuous field theory, the grid spacing must be smaller than the macroscopic length scales of the system like the thermal wavelength and the healing length.

In this paper, we assume that the gas is at thermal equilibrium at temperature T in the canonical ensemble so that the unnormalized density operator is $\rho_{eq}(\beta) = e^{-\beta\mathcal{H}}$ with $\beta = 1/k_B T$. It is a well-known fact of quantum statistical mechanics that this density operator can be obtained as the result of an imaginary-time evolution:

$$\frac{d\rho_{eq}(\tau)}{d\tau} = -\frac{1}{2} [\mathcal{H} \rho_{eq}(\tau) + \rho_{eq}(\tau) \mathcal{H}]. \quad (2)$$

during a “time” interval $\tau = 0 \rightarrow \beta$ starting from the infinite temperature value $\rho_{eq}(\tau = 0) = \mathbf{1}_N$. We have recently shown [12] that the solution of the imaginary-time evolution (2) can be written exactly as a statistical average of Hartree operators of the form

$$\sigma = |N : \phi_1\rangle\langle N : \phi_2| \quad (3)$$

where, in both the bra and the ket, all N atoms share the same (not necessarily normalized) wave functions ϕ_α ($\alpha = 1, 2$). For the model Hamiltonian (1) here considered, this holds if each ϕ_α evolves according to the Ito stochastic differential equations:

$$d\phi_\alpha(\mathbf{r}) = -\frac{d\tau}{2} \left[\frac{p^2}{2m} + U_{\text{ext}}(\mathbf{r}) + g_0(N-1) \frac{|\phi_\alpha(\mathbf{r})|^2}{\|\phi_\alpha\|^2} - \frac{g_0(N-1)}{2} \frac{\sum_{\mathbf{r}'} dV |\phi_\alpha(\mathbf{r}')|^4}{\|\phi_\alpha\|^4} \right] \phi_\alpha(\mathbf{r}) + dB_\alpha(\mathbf{r}) \quad (4)$$

with a noise term given by

$$dB_\alpha(\mathbf{r}) = i\sqrt{\frac{d\tau g_0}{2V}} \mathcal{Q}_\alpha[\phi_\alpha(\mathbf{r}) \sum_{\mathbf{k}>0} (e^{i(\mathbf{k}\cdot\mathbf{r}+\theta_\alpha(\mathbf{k}))} + \text{c.c.})] \quad (5)$$

where the projector \mathcal{Q}_α projects orthogonally to ϕ_α , the index \mathbf{k} is restricted to a half space and the $\theta_\alpha(\mathbf{k})$ are independent random angles uniformly distributed in $[0, 2\pi]$.

Starting from this very simple but exact stochastic formulation, a Monte Carlo code was written in order to numerically solve the stochastic differential equation (4). As a first step, a sampling of the infinite temperature density operator has to be performed in terms of a finite number of random wave functions $\phi^{(i)}$. Since the effective contributions of the different realizations to the final averages can be enormously different, the statistics of the Monte Carlo results can be improved by using an *importance sampling* technique [8] so to avoid wasting computational time. This is done using the identities

$$\mathbf{1}_N = \int_1 \mathcal{D}\phi |N : \phi\rangle\langle N : \phi| = \int_1 P_0[\phi] \mathcal{D}\phi \frac{|N : \phi\rangle\langle N : \phi|}{P_0[\phi]} \quad (6)$$

where the integration is performed over the unit sphere $\|\phi\|^2 = \langle\phi|\phi\rangle = \sum_{\mathbf{r}} dV |\phi|^2 = 1$ and where the *a priori* distribution function $P_0[\phi]$ can be freely chosen in order to maximize the efficiency of the calculation. For the numerical calculations here reported, the following $P_0[\phi]$ has been used

$$P_0[\phi] = \left\| e^{-h_{GP}\beta/2} |\phi\rangle \right\|^{2N} \quad (7)$$

since it joined the possibility of a simple sampling with a fast convergence. In this expression, h_{GP} is the Gross-Pitaevskii Hamiltonian $h_{GP} = \frac{p^2}{2m} + U_{\text{ext}}(\mathbf{r}) + N g_0 |\phi_0(\mathbf{r})|^2 - \mu$, ϕ_0 is the wave function which minimises

the Gross-Pitaevskii energy functional and μ is the corresponding chemical potential. With respect to the ideal Bose gas distribution function previously used [12], the present form (7) for $P_0[\phi]$ has the advantage of taking into account the fact that the condensate mode can be strongly modified by interactions. More details on the actual sampling of $P_0[\phi]$ can be found in [12].

Each realization $\phi_{1,2}^{(i)}$ is then let evolve according to the stochastic evolution in imaginary-time (4) from its $\tau = 0$ value $\phi_{1,2}^{(i)} = \phi^{(i)}$ to the inverse temperature of interest $\tau = \beta$. The expectation values of any observable at temperature T can then be calculated as averages over the Monte Carlo realizations; e.g., the partition function $\text{Tr}[\rho]$ is given by $\text{Tr}[\rho] = \overline{\langle\phi_2|\phi_1\rangle^N}$. In particular, the condensate wavefunction $\phi_{\text{BEC}}(\mathbf{r})$ is the eigenvector of the one-body density matrix

$$\langle \hat{\Psi}^\dagger(\mathbf{r}') \hat{\Psi}(\mathbf{r}) \rangle = \frac{1}{\text{Tr}[\rho]} \overline{\phi_1(\mathbf{r}) \phi_2^*(\mathbf{r}') \langle\phi_2|\phi_1\rangle^{N-1}} \quad (8)$$

corresponding to the largest eigenvalue, that is to the largest mean occupation number [15]. The complete probability distribution $P(N_0)$ for the occupation statistics of the condensate mode is obtained *via* the expression $P(N_0) = \text{Tr}[\hat{\mathcal{P}}_{N_0}\rho] \text{Tr}[\rho]^{-1}$ where $\hat{\mathcal{P}}_{N_0}$ projects onto the subspace in which the condensate mode contains exactly N_0 atoms; in terms of the ansatz (3), the expectation value of the projector can be written as

$$\text{Tr}[\hat{\mathcal{P}}_{N_0}\rho] = \frac{N!}{N_0!(N-N_0)!} \overline{(c_2^* c_1)^{N_0} \langle\phi_2^\perp|\phi_1^\perp\rangle^{N-N_0}} \quad (9)$$

where we have split $\phi_\alpha(\mathbf{r})$ as $c_\alpha \phi_{\text{BEC}}(\mathbf{r}) + \phi_\alpha^\perp(\mathbf{r})$ with $\phi_\alpha^\perp(\mathbf{r})$ orthogonal to the condensate wavefunction.

In fig.1-3 we have summarized the results of the Monte Carlo calculations for a one-dimensional, harmonically trapped gas with repulsive interactions. In fig.1, we have plotted the condensate wavefunction density profile $|\phi_{\text{BEC}}(x)|^2$ for different values of the temperature, see solid lines. As the temperature decreases, the enhanced atomic density at the center of the cloud gives a stronger repulsion among the condensate atoms and therefore a wider condensate wavefunction. In this low temperature regime, we have found a good agreement between the Monte Carlo results and the Bogoliubov prediction for the condensate wavefunction including the first correction to the Gross-Pitaevskii equation due to the presence of non-condensed atoms [16], see dashed lines in fig.1. This was expected, since the numerical examples in this paper are in the weakly interacting regime $n\xi \approx 15 \gg 1$, where n is the density at the trap center and $\xi = (\hbar^2/2mg_0n)^{1/2}$ is the corresponding healing length. For high temperatures, the wavefunction $\phi_{\text{BEC}}(x)$ tends to the harmonic oscillator ground state.

The wavefunction $\phi_{\text{BEC}}(x)$ can then be used to determine the occupation statistics of the condensate mode *via* (9). The signature of Bose condensation is apparent in fig.2: the occupation statistics of the condensate

mode at high temperatures has the same shape as a non-interacting, thermally occupied mode, its maximum value being at $N_0 = 0$. For decreasing T , $P(N_0)$ radically changes its shape; at low T , its maximum is at a non-vanishing value of N_0 and its shape is strongly asymmetric with a longer tail going towards the lower N_0 values, as already noticed in the mean-field approach of [5]. This transition resembles the one occurring in a laser cavity for a pumping rate which goes from below to above threshold [17].

For even lower values of the temperature, see fig.3, most of the atoms are in the condensate and the probability distribution $P(N_0)$ tends to concentrate around values of N_0 close to N . However, interactions prevent the atomic sample from being totally Bose condensed even at extremely low temperatures. Moreover, the probability of having an odd number of non-condensed atoms is strongly reduced with respect to the probability of having an even number (see the strong oscillations in the $k_B T = 0.4 \hbar \omega$ curve of fig.3). A quantitative interpretation of this effect in terms of the Bogoliubov approximation will be given in the following part of the paper.

We now compare the exact results with the prediction of the number-conserving Bogoliubov approximation [16, 18]. The Bogoliubov Hamiltonian has the form

$$\mathcal{H}_{\text{Bog}} = \frac{1}{2} dV \left(\vec{\Lambda}^\dagger, \vec{\Lambda} \right) \cdot \eta \mathcal{L} \begin{pmatrix} \vec{\Lambda} \\ \vec{\Lambda}^\dagger \end{pmatrix} \quad (10)$$

with

$$\mathcal{L} = \begin{pmatrix} h_{\text{GP}} + \mathcal{Q}_0 N g |\phi_0|^2 \mathcal{Q}_0 & \mathcal{Q}_0 N g \phi_0^2 \mathcal{Q}_0^* \\ -\mathcal{Q}_0^* N g \phi_0^{*2} \mathcal{Q}_0 & -h_{\text{GP}} - \mathcal{Q}_0^* N g |\phi_0|^2 \mathcal{Q}_0^* \end{pmatrix}. \quad (11)$$

The matrix η is defined according to

$$\eta = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} \quad (12)$$

and the projector \mathcal{Q}_0 projects orthogonally to the Gross-Pitaevskii ground state ϕ_0 . The operators $\vec{\Lambda}$ are defined according to $(\vec{\Lambda})_{\mathbf{r}} = \hat{\Lambda}_0^\dagger \hat{\Psi}_\perp(\mathbf{r})$ where $\hat{\Psi}_\perp(\mathbf{r})$ is the projection of the field operator orthogonally to ϕ_0 and where $\hat{A}_0 |N_0; \phi_0\rangle = |N_0 - 1; \phi_0\rangle$ if $N_0 > 0$ and 0 otherwise. Neglecting the possibility of completely emptying the condensate mode, \hat{A}_0 and \hat{A}_0^\dagger can be shown to commute. Under this approximation, the $\vec{\Lambda}$ are bosonic operators. The probability $\Pi(\delta N)$ of having δN non-condensed atoms can be calculated within the Bogoliubov approximation by means of the characteristic function [4]

$$f(\theta) = \sum_{\delta N} \Pi(\delta N) e^{i \delta N \theta} \simeq \text{Tr} \left[e^{i \theta \delta \hat{N}} \frac{1}{\mathcal{Z}} e^{-\beta \mathcal{H}_{\text{Bog}}} \right] \quad (13)$$

with $\delta \hat{N} = dV \vec{\Lambda}^\dagger \cdot \vec{\Lambda}$ and $\mathcal{Z} = \text{Tr} [e^{-\beta \mathcal{H}_{\text{Bog}}}]$; when the probability of emptying the condensate mode is not totally negligible, the Bogoliubov prediction for $\Pi(\delta N)$ has

to be truncated to the physically relevant $\delta N \leq N$ values and then renormalized to 1. The details of the calculation will be given elsewhere, we go here to the result

$$f(\theta) \simeq \prod_{j=1}^{2(\mathcal{N}-1)} \left[\frac{2\lambda_j}{1 + \lambda_j - e^{i\theta}(1 - \lambda_j)} \right]^{1/2} \quad (14)$$

in which the λ_j are the eigenvalues of $\mathcal{M} = \eta \tanh(\beta \mathcal{L}/2)$; from such an expression, the occupation probabilities $\Pi(\delta N)$ are immediately determined by means of an inverse Fourier transform. The results are shown as dashed lines in figs.2 and 3 where they are compared to the exact results from Monte Carlo simulations; the agreement is excellent provided the non-condensed fraction is small, i.e. at sufficiently low temperatures.

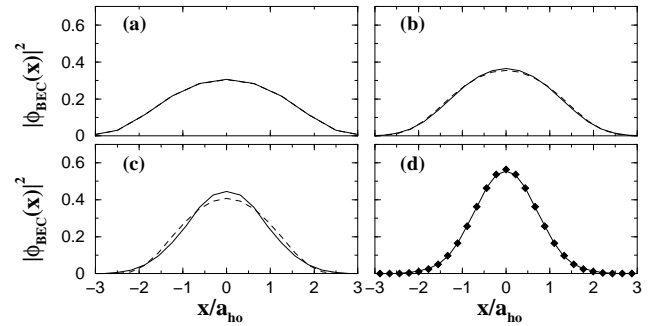


FIG. 1: Solid lines: exact results for the condensate wavefunction density profile $|\phi_{\text{BEC}}(x)|^2$ for $N = 125$ atoms in a one-dimensional harmonic trap at different temperatures $k_B T / \hbar \omega = 1$ (a), 10 (b), 20 (c), 50 (d). ω is the trap frequency, $|\phi_{\text{BEC}}|^2$ is in units of the inverse of $a_{\text{ho}} = \sqrt{\hbar/m\omega}$. The coupling constant is $g_0 = 0.08 \hbar \omega a_{\text{ho}}$. Comparison with Bogoliubov predictions (dashed lines) in (a,b,c) and with harmonic oscillator ground state (diamonds) in (d). In (a) the two lines are indistinguishable on the scale of the figure. Monte Carlo calculations were performed using $3 \cdot 10^4$ realisations on a $\mathcal{N} = 16$ (a), 64 (b,c) or 128 point (d) grid.

In order to understand the oscillating behaviour shown by the lowest temperature curve of fig.3, we calculate the ratio of the probability Π_{odd} of having an odd value of δN to the probability Π_{even} of having an even value:

$$\frac{\Pi_{\text{odd}}}{\Pi_{\text{even}}} = \frac{f(0) - f(\pi)}{f(0) + f(\pi)} \simeq \frac{1 - R}{1 + R} \quad (15)$$

where $R = \prod_j \lambda_j^{1/2} = \det[\mathcal{M}]^{1/2} = \prod_m \tanh(\beta \epsilon_m/2)$ and m runs over the $\mathcal{N}-1$ eigenenergies ϵ_m of the Bogoliubov spectrum. In order to have oscillations in $\Pi(\delta N)$, the ratio (15) must be small as compared to 1 which requires a temperature smaller than the energy of the lowest Bogoliubov mode. These oscillations are therefore a property of the ground state of the system. In the Bogoliubov approximation, the Hamiltonian is quadratic in the field operators so that its ground state is a squeezed vacuum, which indeed contains only even values of δN , a well known fact of quantum optics [19]. From a condensed

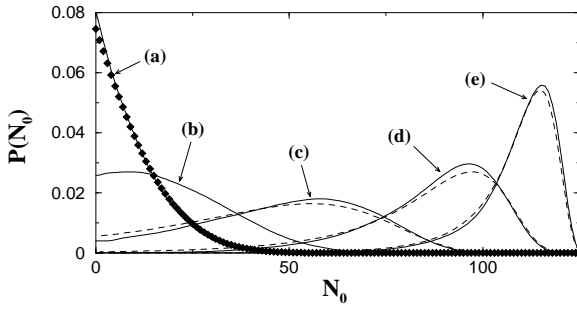


FIG. 2: Solid lines: exact results for the distribution function $P(N_0)$ of the number of condensate atoms for decreasing temperatures from left to right: $k_B T / \hbar \omega = 50$ (a), 33 (b), 20 (c), 10 (d), 5 (e). Same parameters as in fig.1. For curves (c,d,e), comparison with Bogoliubov predictions (dashed lines); for curve (a), comparison with the ideal gas (diamonds). The Monte Carlo calculations were performed using $3 \cdot 10^4$ realisations on a grid of $\mathcal{N} = 128$ (a,b) or $\mathcal{N} = 64$ points (c,d,e).

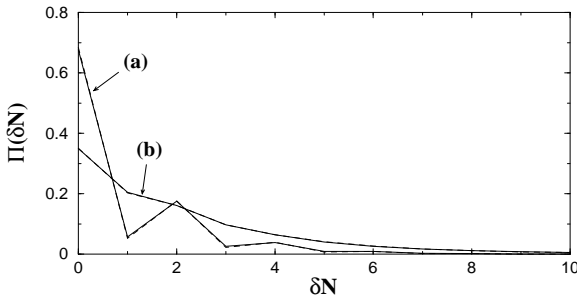


FIG. 3: Solid lines: exact results (10^5 realizations on a $\mathcal{N} = 16$ point grid) for the distribution function $\Pi(\delta N) = P(N_0 = N - \delta N)$ of the number of non-condensed atoms at low temperatures $k_B T / \hbar \omega = 0.4$ (a) and 1 (b). Same parameters as in fig.1 and fig.2. Dashed lines: Bogoliubov predictions. For $k_B T / \hbar \omega = 0.4$, the two lines are indistinguishable on the scale of the figure.

matter point of view, several existing variational ansatz for the ground state corresponding to a condensation of pairs also exhibit this property [20, 21]. Physically, this is ultimately related to the fact that the leading interaction process changing the condensate occupation at zero temperature, that is the scattering of two condensate particles into two non-condensed modes and *vice-versa*, does not change the parity of δN , as it is apparent in the Bogoliubov Hamiltonian (10).

In conclusion, we have determined with a newly developed stochastic field Quantum Monte Carlo method the exact distribution function of the number N_0 of condensate particles in a one-dimensional weakly interacting trapped gas. The signature of Bose condensation is the appearance of a finite value for the most probable

value of N_0 . At temperatures below the trap oscillation frequency, configurations with an odd number of non-condensed particles are strongly suppressed, which we interpret successfully within the Bogoliubov approximation. Possible extensions of this work are (i) the determination of critical temperature shift for an interacting Bose gas in the limit of a vanishing scattering length, still subject of some controversy [22], (ii) exact calculations for finite temperature Bose gases with vortices in rotating traps, and (iii) the determination of the BCS critical temperature in two-component Fermi gases.

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